An optimization-based, positivity-preserving spherical harmonic closure for linear, kinetic transport equations.

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January 30, 2009

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Outline

The P_N Equations

Kinetic Description of Particle Systems

We considered a particle distribution described at the kinetic level by a **kinetic distribution function** (or **kinetic density** or **angular flux**) $F = F(x, \Omega, t)$, which gives the number of particles

- At position $x \in \mathbb{R}^3$,
- Traveling in direction $\Omega \in \mathbb{S}^2$,
- And time $t \geq 0$.
- For simplicity, we assume
  - Particles scatter isotropically off a background material medium, characterized a **scattering cross-section** $\sigma = \sigma(x)$.
  - Particles are mono-energetic, with speed $|v|$=1

The Transport Equation

- The evolution of $F = F(x, \Omega, t)$ is governed by a kinetic **transport equation**:

$$\boxed{\partial_t F + \Omega \cdot \nabla_x F + \sigma F = \frac{\sigma}{4\pi}\langle F \rangle.}$$

- Notation: Angle brackets denote integration of the angular variable over the sphere $\mathbb{S}^2$.
- An important quantity of is $\phi = \langle F \rangle$, the **concentration** (or **density** or **scalar flux**), which is conserved:

$$\boxed{\partial_t \phi + \nabla_x \cdot \langle \Omega F \rangle = 0\,.}$$

Moment Equations

- Let $\mathbf{p} = \mathbf{p}(\Omega)$ be a vector of functions of Ω.
- Let $\mathbf{u}(x,t) := \langle \mathbf{p} F(x,\Omega,t) \rangle$ be moments of F with respect to $\mathbf{p}$.
- To derive moment equations, multiply the transport equation by $\mathbf{p}$ and integrate over all angles:

$$\boxed{\partial_t \mathbf{u} + \nabla_x \cdot \langle \Omega \mathbf{p} F \rangle + \sigma \langle \mathbf{p} F \rangle = \frac{\sigma}{4\pi} \langle \mathbf{p} \rangle \phi \,.}$$

- To close the system, one must prescribe an ansatz to approximate F—

$$\boxed{F(x,\Omega,t) \simeq \mathcal{F}(\mathbf{u}(x,t),\Omega)}$$

—that satisfies the **consistency relation**

$$\boxed{\langle \mathbf{p} \mathcal{F}(\mathbf{u}(x,t),\cdot) \rangle = \mathbf{u} \,.}$$

The Spherical Harmonic (or P_N) Closure

- For the P_N closure:
  - Components of $\mathbf{p}$ are spherical harmonic polynomials up to degree N.
  - The reconstruction $\mathcal{F}$ is a linear combination of components of $\mathbf{p}$:

$$\boxed{\mathcal{F}(\mathbf{u}(x,t),\Omega) = \mathbf{c}(x,t)^T\mathbf{p}}$$

- Consistency relation implies:

$$\boxed{\mathbf{u} = \left\langle \mathbf{p}\mathbf{p}^T \right\rangle \mathbf{c}\,.}$$

- The zeroth order moment is just ϕ:

$$\boxed{\partial_t \phi + \nabla_x \cdot \langle \Omega \mathcal{F} \rangle = 0\,.}$$

Negative Solutions

Negative Solutions

- What is known?
  1. Solutions F to the transport equation are non-negative.
  2. Solutions to the P_N equations in 1-D have positive particle concentrations.
  3. Solutions to the P_N equations in multi-D can have negative particle concentrations.

- Insight can be gained even from the one-dimensional setting.

Analysis in One Dimensional, Slab Geometries

- Decompose Ω into Cartesian components: $\Omega = (\mu, \eta, \zeta)^T$
- In **slab geometries** $F = F(x, \mu, t)$ satisfies

$$\boxed{\partial_t F + \mu \partial_x F + \sigma F = \frac{\sigma}{2}\phi\,.}$$

- The angular variable $\mu \in [-1, 1]$ is the cosine between the x-axis and the direction of particle travel
- Notation: Angled brackets in 1-D denote integration over μ.

The P_N Equations in One Dimension

- The P_N equations take the form

$$\boxed{\partial_t \mathbf{u} + A\partial_x \mathbf{u} = -\sigma Q\mathbf{u}}$$

where the **flux matrix** A and the **relaxation matrix** Q are given by

$$\boxed{\begin{aligned} A_{nm} &= \frac{n+1}{2n+1}\,\delta_{n+1,m} + \frac{n}{2n+1}\,\delta_{n-1,m} \\ Q_{nm} &= \delta_{nm}(1-\delta_{n,0}) \end{aligned}}$$

- A is diagonalizable: $A = L\Lambda R$. Eigenvalues $\{\lambda_0 \cdots \lambda_N\}$ form the $N+1$-point Gauss-Legendre quadrature set.

Discrete Ordinate Formulation

- A particular choice of right and left eigenvectors diagonalizes the P_N equations into an equivalent discrete ordinate form:

$$\boxed{\partial_t \mathbf{w} + \Lambda \partial_x \mathbf{w} + \sigma \mathbf{w} = \frac{\sigma}{2} \mathbf{e} \phi \,,}$$

where $\mathbf{e} = [1, \ldots, 1]^T$.

- The n-th component of $\mathbf{w}$ is a solution to the transport equation along the direction $\mu = \lambda_n$, but with initial condition

$$\boxed{\mathcal{F}(x, \mu, 0) = \mathbf{c}^T(x, 0)\mathbf{p}(\mu) = \left\langle \mathbf{p}\mathbf{p}^T \right\rangle^{-1} \left\langle \mathbf{p}^T F(x, \cdot, 0) \right\rangle \mathbf{p}(\mu) \,.}$$

Discrete Ordinate Formulation

- Density is a weighted sum of components of **w**:

$$\phi = \boldsymbol{\alpha}^T \mathbf{w}\,, \tag{1}$$

where components of $\boldsymbol{\alpha}$ are Gauss-Legendre quadrature weights.

A Semi-Implicit, Upwind (SIU) Scheme

- First order, semi-implicit method based on upwinding:

$$\boxed{\begin{aligned}\mathbf{w}_j^{s+1} = \mathbf{w}_j^s - \Delta t \Lambda^+ \left(\frac{\mathbf{w}_j^s - \mathbf{w}_{j-1}^s}{\Delta x} \right) \\ + \Delta t \Lambda^- \left(\frac{\mathbf{w}_{j+1}^s - \mathbf{w}_j^s}{\Delta x} \right) - \Delta t \sigma \left(\mathbf{w}_j^{s+1} - \mathbf{e} \phi_j^{s+1} \right)\end{aligned}}$$

- In terms of the moments:

$$\boxed{\begin{aligned}\mathbf{u}_j^{s+1} = \mathbf{u}_j^s - \Delta t A \left(\frac{\mathbf{u}_{j+1}^s - \mathbf{u}_{j-1}^s}{2\Delta x} \right) \\ - \Delta t |A| \left(\frac{\mathbf{u}_{j+1}^s - 2\mathbf{u}_j^s + \mathbf{u}_{j-1}^s}{2\Delta x} \right) - \Delta t \sigma \mathbf{u}^{s+1}\end{aligned}}$$

where $|A| = L|\Lambda|R$ and $\Lambda^\pm = \frac{1}{2}(\Lambda \pm |\Lambda|)$.

Positivity Preserving Property

Proposition

The SIU scheme preserves the positivity of the components of $\mathbf{w}$ *and the density* ϕ *under the CFL condition* $\Delta t < \Delta x$.

However, this result says nothing about the angular reconstruction for values of $\mu \neq \lambda_n$.

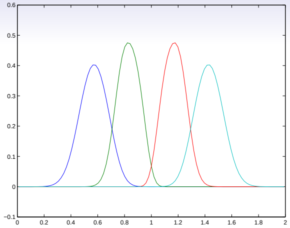
Numerical Example: the P_3 System

Apply SIU algorithm to a test problem with:

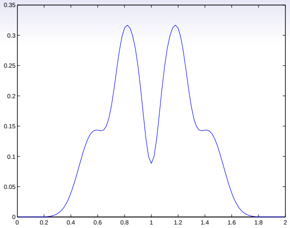
- Periodic boundary conditions.
- Initial condition for ϕ is

$$\boxed{\phi(x,0) = \begin{cases} 2.0, & x \in (0.8, 1.2)\ , \\ 0.0, & x \in [0, 0.8] \cup [1.2, 2.0]\ , \end{cases}}$$

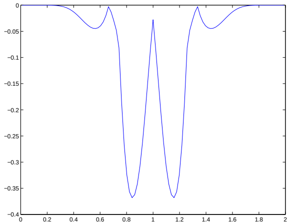
- All other moments are initially zero.



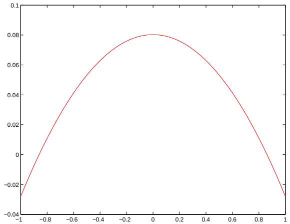
(a) Components of $\mathbf{w}$



(b) Concentration, ϕ



(c) $\min_{\mu \in [-1,1]} \mathcal{F}(\mathbf{u}(x,1),\mu)$



(d) Angular reconstruction at $x = 1$.

Figure: P_3 Results

The Positive-Preserving Closure

Variational Formulation of the P_N Closure

- The P_N closure can also be formulated as the solution to the following optimization problem

$$\boxed{\begin{array}{rl} \text{minimize} & \dfrac{1}{2}\left\langle |f|^2 \right\rangle \\ \text{subject to} & \langle \mathbf{p} f \rangle = \langle \mathbf{u} \rangle \end{array}}$$

A New, Modified Closure

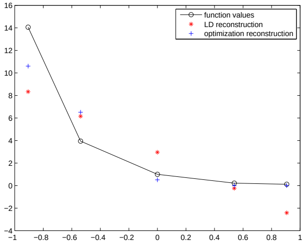
- IDEA: Modify the P_N closure by adding an inequality constraint to the optimization problem

$$\boxed{\begin{array}{rl} \text{minimize} & \frac{1}{2}\left\langle |f|^2 \right\rangle \\ \text{subject to} & \langle \mathbf{p} f \rangle = \langle \mathbf{u} \rangle \ , \ f \geq 0 \end{array}}$$

- Enforcing positivity everywhere is not possible. Discretize the problem on a quadrature set $\mathcal{Q} \in [-1, 1]$:

$$\boxed{\begin{array}{rl} \text{minimize} & \displaystyle \frac{1}{2} \sum_{\Omega_k \in \mathcal{Q}} \omega_k [f(\Omega_k)]^2 \\ \text{subject to} & \displaystyle \sum_{\Omega_k \in \mathcal{Q}} \omega_k \mathbf{p}(\Omega_k) f(\Omega_k) = \langle \mathbf{u} \rangle \ , \ f(\Omega_k) > 0 \ \forall \ \Omega_k \in \mathcal{Q} \end{array}}$$

The Optimization



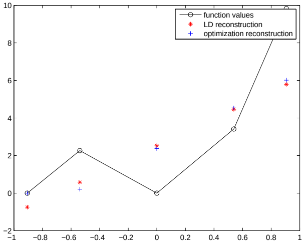


Figure: Example optimization output.

Initial Implementation: 1-D

Kinetic Scheme

- Challenge: Ensure positivity is not destroyed by the scheme.
  of cells $I_i = [x_{i-1/2}, x_{i+1/2}]$ of width Δx.
- Semi-discrete, finite volume formulation:

$$\boxed{\partial_t F_i + \mu \frac{F_{i+1/2} - F_{i-1/2}}{\Delta x} + \sigma F_i = \frac{\sigma}{2}\phi_i}$$

Kinetic Scheme

- Determine pointwise edges values with upwinding

$$\boxed{\begin{aligned}\partial_t F_{i,k} + \max(\mu^k, 0)\frac{F_{i,k} - F_{i-1,k}}{\Delta x} \\ + \min(\mu^k, 0)\frac{F_{i+1,k} - F_{i,k}}{\Delta x} + \sigma F_{i,k} = \frac{\sigma}{2}\phi_i\end{aligned}}$$

- Apply the quadrature, using the equality constraints to evaluate the moments and relaxation terms:

$$\boxed{\partial_t \mathbf{u}_i + \sum_{\mu_k > 0} \omega_k \frac{F_{i,k} - F_{i-1,k}}{\Delta x} + \sum_{\mu_k < 0} \omega_k \frac{F_{i+1,k} - F_{i,k}}{\Delta x} = Q\mathbf{u}_i}$$

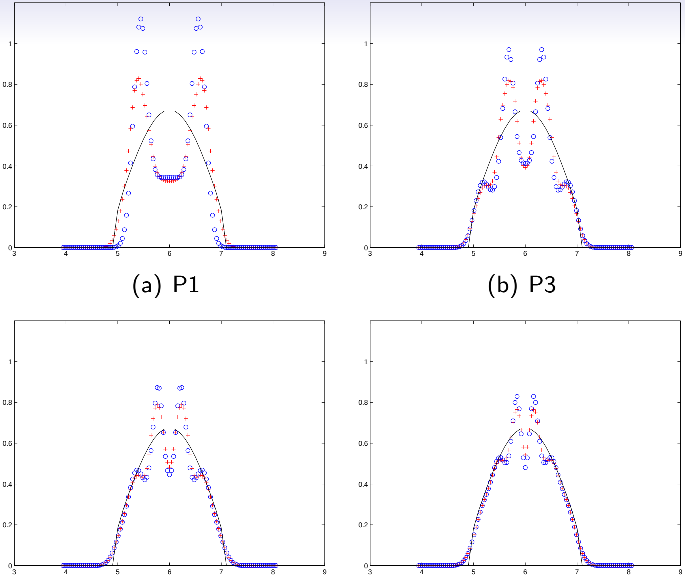
Properties of the Algorithm

- GOOD:
  1. Closure is local.
  2. Reverts back to standard P_N when positivity is not violated.

- BAD
  1. Only first-order.
  2. NOT asymptotic preserving.

Numerical Example: Pulse in One Dimension

- Periodic boundary conditions.
- Density ϕ is initially a delta function at $x = 1$.
- All other moments initially zero.



(a) P1 (b) P3

(c) P5 (d) P7

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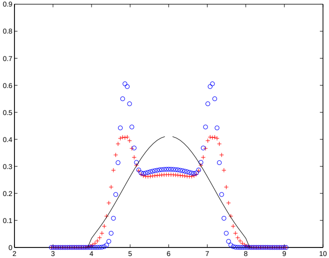
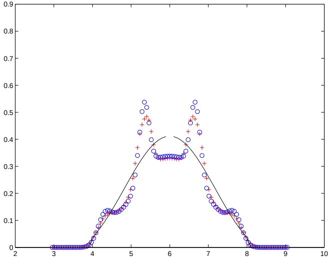
Figure: Results, 1-D Pulse, $t = 1.0$.

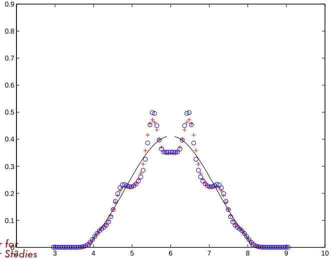
1-D Pulse Results



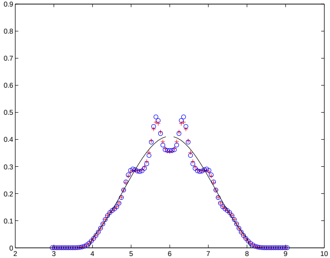
(a) P1



(b) P3

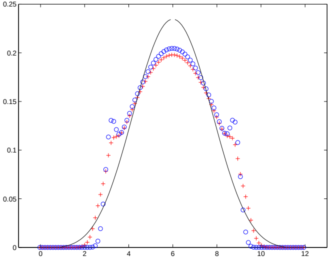


(c) P5

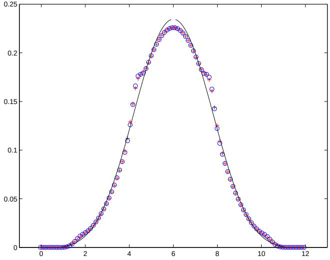


(d) P7

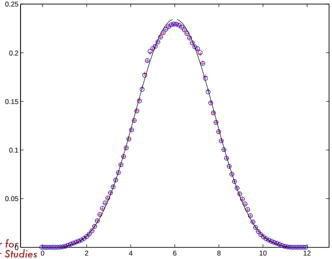
1-D Pulse Results



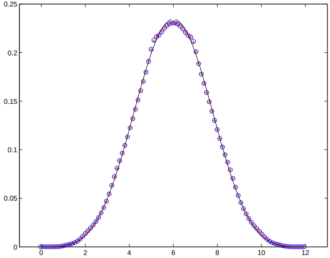
(a) P1



(b) P3



(c) P5



(d) P7

Initial Implementation: 2-D

Implementation: 2-D

- Recall $\Omega = [\mu, \eta, \zeta]^T$.
- In two dimensions, the transport equation is

$$\boxed{\partial_t F + \mu \partial_x F + \eta \partial_y F + \sigma F = \frac{\sigma}{4\pi} \phi}$$

- Choose a quadrature set Q and evolve F along directions $\mu_k, \eta_k \in \mathcal{Q}$.

Implementation: 2-D

- A first-order, finite volume:

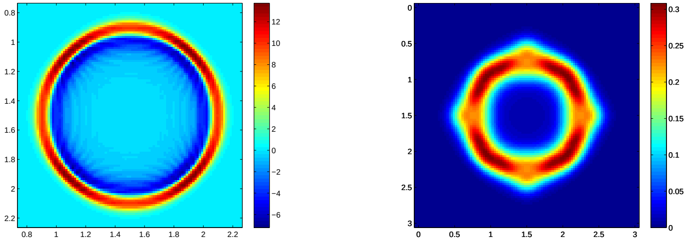
$$\boxed{\begin{aligned}\partial_t F_{i,j,k} &+ \max(\mu_k,0)\frac{F_{i,j,k}-F_{i-1,j,k}}{\Delta x} + \min(\mu_k,0)\frac{F_{i+1,j,k}-F_{i,j,k}}{\Delta x} \\ &+ \max(\eta_k,0)\frac{F_{i,j,k}-F_{i,j-1,k}}{\Delta y} + \min(\eta_k,0)\frac{F_{i,j+1,k}-F_{i,j,k}}{\Delta y} \\ &+ \sigma_{i,j,k} = \frac{\sigma}{4\pi}\phi_{ij}\end{aligned}}$$

- Integrate this discretization against $\mathbf{p}$; apply constraints:

$$\boxed{\begin{aligned}\partial_t \mathbf{u}_{i,j} &+ \sum_{\mu_k>0,\eta_k} \omega_k \frac{F_{i,j,k}-F_{i-1,j,k}}{\Delta x} + \sum_{\mu_k<0,\eta_k} \omega_k \frac{F_{i+1,j,k}-F_{i,j,k}}{\Delta x} \\ &+ \sum_{\mu_k,\eta_k>0} \omega_k \frac{F_{i,j,k}-F_{i,j-1,k}}{\Delta y} + \sum_{\mu_k,\eta_k<0} \omega_k \frac{F_{i,j+1,k}-F_{i,j,k}}{\Delta y} \\ &= Q\mathbf{u}_{i,j}\end{aligned}}$$

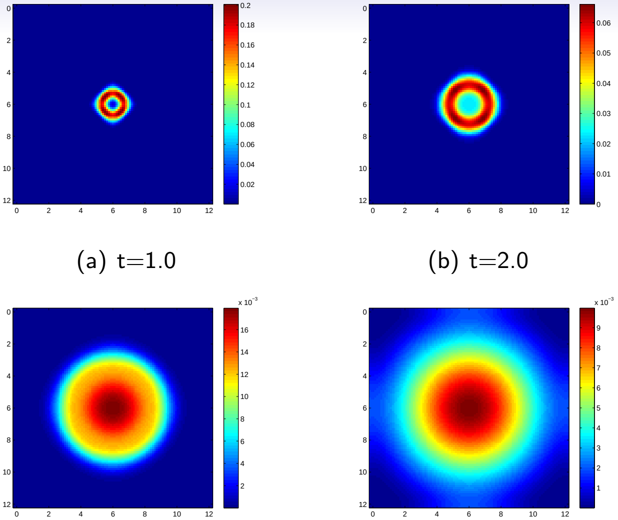
Numerical Example: Line Source in Two Dimension

- Periodic boundary conditions.
- Density ϕ is initially a delta function at $x = y = 0$.
- All other moments initially zero.



(a) standard closure (b) modified closure

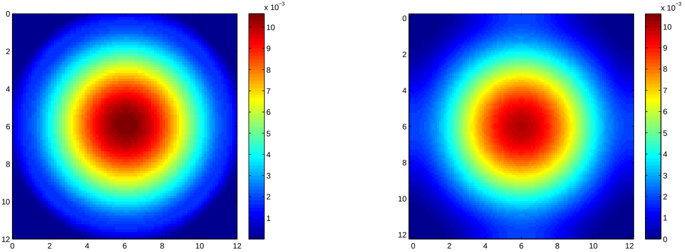
Figure: Linesource Problem, $t = 1.0$.



(a) t=1.0 (b) t=2.0

(c) t=5.0 (d) t=10.0

Figure: Linesource Problem, $t = 1.0$.



(a) standard closure

(b) modified closure

Figure: Linesource Problem, $t = 10.0$.

Future Work

- Higher Order Discretizations
- Asymptotic Preserving Implementation.
- Parallelization.

Acknowledgments

- Center for Nonlinear Studies, Los Alamos.
- DOE, Advanced Scientific Computing Research.